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May 12, 1997

To whom it may concern:

We have successfully completed the research project "An x-ray analysis database of photoionization cross sections including variable ionization", which is the contracted work under the contract NAS5-32646. Attached is the final report of the work. Let me know if you have any questions about this project.

Sincerely,

Ping Wang

Ping Wang

An X-Ray Analysis Database of Photoionization Cross Sections Including Variable Ionization

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(1) Introduction

In this report we summarize work performed at the University of Wisconsin Fusion Technology Institute under the NASA contract NAS5-32646. This work has focussed on:

- Reviewing the major theoretical and experimental data of subshell photoionization cross sections and ionization edges of atomic ions previously published to assess the accuracy of the data, and to compile the most reliable of these data in our own data base.
- Doing detailed atomic physics calculations to complement the data base for all ions of 17 cosmically abundant elements.
- Reconciling the data from various sources and our own calculations.
- Fitting cross sections with functional approximations and incorporating these functions into a compact computer code.
- Adapting an ionization equilibrium code, tabulating results, and incorporating them into the overall program.
- Testing the code (both ionization equilibrium and opacity codes) with existing observational data.

The results of this work are discussed in the report as follows. In Section 2, we discuss the background and scientific applications of this work. In Section 3, atomic physics cross section models and calculations are described. Our calculation results are also compared with available experimental data and other theoretical data. In Section 4, we outline the functional approximations we used for fitting cross sections. Finally, in Section 5, we discuss the applications of our database.

(2) The Scientific Background and Applications of This Work

Correcting for attenuation that occurs between the source and the observer is a crucial aspect of many studies of X-ray emission. At the present time this is being done

using simple opacity routines that assume the intervening medium is neutral or treats the directed opacity of ionized material by putting a low-energy "window" in the neutral cross sections. Alternatively, some researchers do complex ionization modeling off-line and then read tabulated cross sections into data fitting routines. In this method, however, the opacities are *fixed* for the data fitting. While these may be useful first steps, our increasing awareness of ionization conditions in many astrophysical contexts and the higher quality of the available X-ray data demands a greater degree of flexibility on the part of the observer. In particular, with the improved spectral resolution and calibration of the next generation of instruments (ASTRO·E, XMM, and AXAF) it is becoming possible to test source models with greater degrees of sophistication. This requires a more realistic modeling of the X-ray absorption, but one that is tractable and easy to perform as part of an in-line analysis.

The effect of ionization on photoionization cross sections was investigated by Krolik and Kallman (1984). They point out that there are two effects which lead to changes in the opacities of ionized species. First, as electrons are stripped from an atom, shielding of the nucleus is decreased and the cross section for subsequent K-shell ionization decreases while the threshold energy increases. Second, when atoms become totally ionized they are no longer capable of absorbing a photon at all. The general decrease in opacity with increasing ionization stage is not at all uniform, since the atoms with the lower ionization potentials preferentially absorb soft X-rays. In Figure 1 we show the cross section for cosmically abundant neutral gas along with photoionized plasma appropriate to a hot star wind. Note that even at relatively moderate ionization levels the opacity at low photon energies can be strongly affected. Note also the shift in energy of the K-shell edges of some of the heavy elements, notably the oxygen and carbon edges. Also, because H and He are highly ionized, the L-shells of heavier ions are visible below the carbon K-shell edge.

The interest in modeling is often simply to derive the emission properties of an X-ray source. In these cases absorption is to be corrected for so that the underlying X-ray spectrum can be derived. Here, assuming that the absorbing medium is fully neutral can lead to large errors in the derived properties of the intrinsic X-ray emission. This is especially true for soft X-rays where much of the opacity is provided by hydrogen and neutral helium. However in a hot medium this will lead to problems at higher photon energies as well. From Figure 1 we can clearly see that the X-ray spectral parameters, including the total emitted X-ray flux, may be grossly in error if the standard X-ray attenuation software is blindly used.

The impetus for improving the available software for calculating cross sections is both observational and theoretical. As our understanding of the complexity of AGN's,

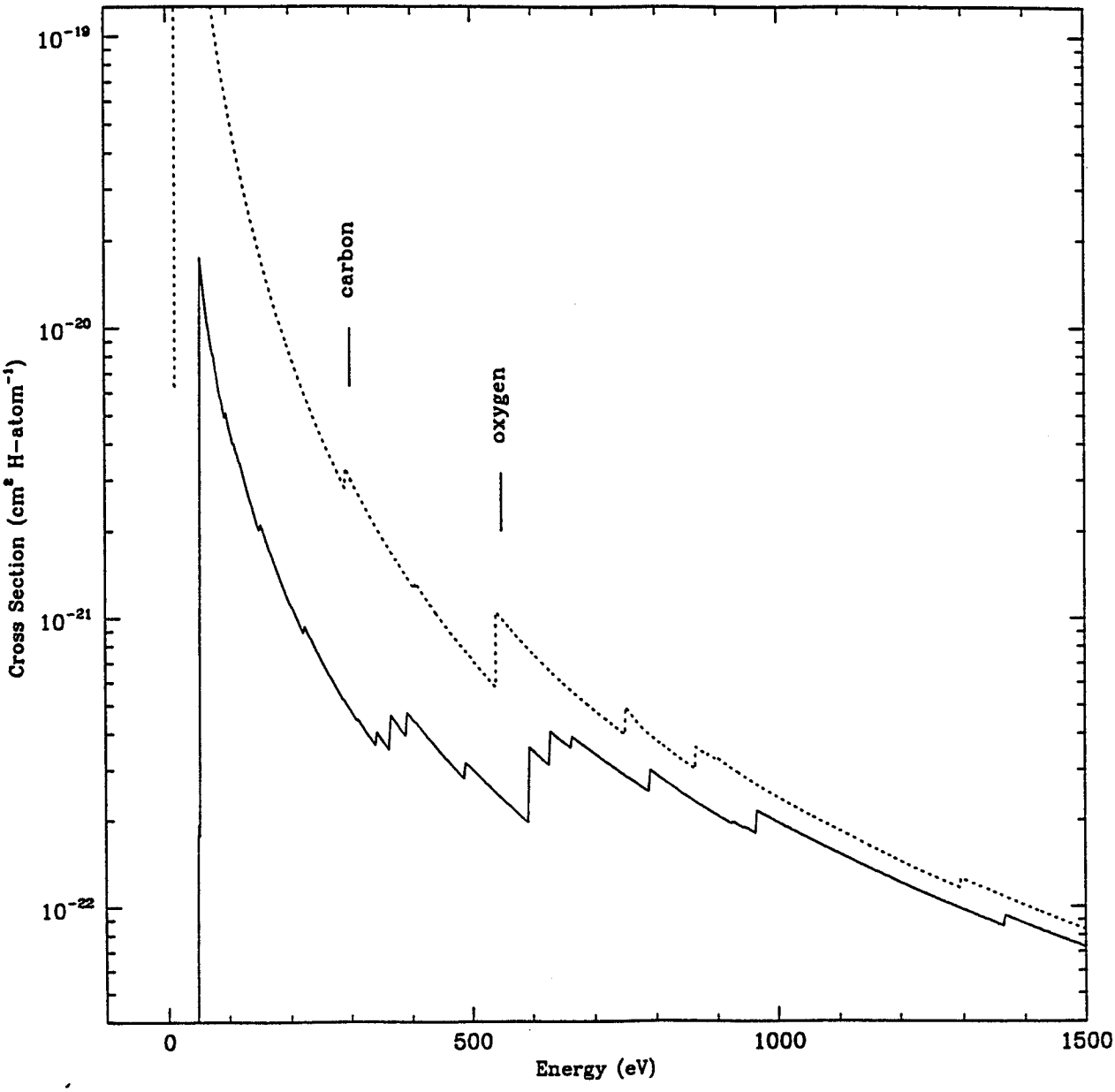

Figure 1. Total cross section for two cosmically abundant plasmas. The dotted line is for a fully neutral plasma and the solid line is for a warm, photoionized hot star wind. Note the large decrease in soft X-ray opacity due primarily to helium ionization. Note also the shifting to higher energies of bound-free edges.

winds, X-ray binaries, and other astrophysical environments grows, it is becoming clear that many of these settings contain highly ionized gas. Along with this enhanced theoretical understanding have come improved X-ray telescopes which have the capability of studying deviations from purely neutral attenuation. ASCA and BBXRT data already in the public archives show the effects of absorption (or lack thereof) by ionized hydrogen, helium, oxygen, and iron.

Individual K-shell edges of oxygen have been included in some BBXRT modeling (Corcoran et al. 1993), although here too there is no standardized software for making a consistent model of X-ray attenuation in ionized media. Indeed these researchers used the K-shell edge cross-sections and threshold energies which were compiled over twenty years ago by Daltabuit and Cox (1972), and included only ions of oxygen in their models. X-ray data from the ASCA satellite is of even higher spectral resolution that BBXRT. Results from ASCA show K-shell edges in some sources, such a Puppis A (Inside Astrophysics, NASA publication, Spring 1993). We have found improved model fits of X-rays EUV data from hot stars using the cross sections discussed in the report (see Section 5).

These issues are not unique to stellar astronomers. In general, any astronomer wishing to model source absorption (i.e. attenuation of X-rays near the site of emission) will need to consider the ionization state of the absorbing medium. This is an issue in studies of novae. Novae ejecta pass through several distinct stages of ionization, including a coronal stage (Williams 1989). Although there are several models for the X-ray emission which imply strong local absorption by ionized gas, X-ray modeling of objects such as Nova Her 1991 has been performed using opacities for neutral gas only (Lloyd et al. 1992). The same is true for AGN's where both warm and hot ($10^6 - 10^7$ K) gas exists in large quantities near the site of X-ray production. Attempts to derive column densities of local absorbing gas have assumed that the gas is neutral (Petre et al. 1984). However, ionization will reduce the opacity, especially at soft photon energies, and this situation must be modeled if accurate column densities of local ionized gas are to be derived from X-ray observations. More recently, warm absorbers have been modeled off-line with detailed codes like CLOUDY (Ferland 1990). Ion balances opacities thus derived are then typically read into fitting programs such as XSPEC or as table files and the fit is then performed with fixed cross sections.

In order to allow astrophysicists to more accurately model the energy-dependent cross sections in ionized media we have developed a code which supplies energy-dependent cross sections of plasma with arbitrary ionization stages and abundances of 17 elements. These values were calculated using the methods described in Section 3 and provide a

convenient way for researchers to obtain cross sections of individual ions or of a plasma with a mixture of many ions for modeling, data analysis, or observing feasibility studies. The set of cross sections, all tabulated in a single code, will also provide an interesting comparison with the values found in the Opacity Project (OP, Seaton 1987), the Hartree-Dirac-Slater (HDS) calculations by Verner et al. (1993), and other older tabulations. We also have developed a compact code to approximate the ionization balances under arbitrary thermal or photoionization conditions. In conjunction with the cross section tabulations this code will allow for the straight forward fitting of X-ray spectra which are attenuated by partially ionized media.

As the quality of astronomical X-ray data improves, not only will researchers want to fit their data with models of partially ionized absorbers, but the accuracy of photoionization cross sections will become more of an issue. Currently, the tabulations of Henke *et al.* (1982) and even Daltabuit and Cox (1972) are commonly used. Recently Verner and Yakovlev (1995) and Verner et al. (1996) have published a large compilation of cross sections, some of which are incorporated in the CLOUDY program. As in any complex scientific undertaking, it is important that researchers have access to quantities that are calculated using a range of modeling techniques. We feel that the discrepancies between the cross sections of Verner and Yakovlev (1995) and those that we have calculated will spur further research into the complex field of atomic modeling.

(3) Atomic Physics Models and Calculations

We have calculated subshell photoionization cross sections of atoms and ions at all ionization states for 17 elements (H, He, C, N, O, Ne, Na, Mg, Al, Si, S, Cl, A, Ca, Cr, Fe, and Ni) with the use of the multiconfiguration Hartree-Fock (HF) method. It is well known that relativistic effects on ionization potentials and radial wavefunctions become appreciable for Z as small as 10 and 30, respectively. We incorporate the major relativistic effects within the format of non-relativistic approach in the same way as that proposed by Cowan (1981). Comparison with available experimental data and other more refined theoretical results show that our calculated ionization potentials and photoionization cross sections are quite accurate for both outer shell and inner shell electrons. In addition, particular efforts have been made to include the many-electron correlation effect in a one-electron approximation. Hence, our calculations give better description for some special photoionization cross section features such as 'Cooper-minimum' which is related to the electron correlation effect than most other one-electron central potential models.

In the one-electron approximation, the wavefunction of an atom can be represented in the form of a determinant made up of one-electron wavefunctions. The atomic subshell photoionization cross section can be expressed as

$$\sigma_{nl}(\epsilon) = \frac{4\pi^2 \alpha a_0^2}{3} \frac{N_{nl}(\epsilon + \epsilon_{nl})}{2l+1} [l R_{l-1}^2 + (l+1) R_{l+1}^2], \tag{1}$$

where σ is in cm^2, α is the fine-structure constant, a_0 is the Bohr radius, N_{nl} is the number of electron in the nl subshell, ϵ_{nl} is the binding energy of the electron in the nl subshell (in atomic units), and ϵ is the kinetic energy of the ionized electron, and $R_{l\pm1}(\epsilon)$ are one-electron radial dipole matrix elements:

$$R_{l\pm1} = \int_0^\infty P_{nl}(r) r P_{\epsilon,l\pm1}(r) dr\,, \tag{2}$$

where $P_{nl}(r)$ and $P_{\epsilon,l\pm1}(r)$ are the bound (initial) and the continuum (final) single-particle radial wavefunctions.

In the one-electron approximation, the accuracy of the calculated photoionization cross sections depends entirely on how accurate the wavefunctions are. In our calculations, the bound state wavefunctions $P_{nl}(r)$ are calculated with the use of the Hartree-Fock method. The wavefunctions of the outgoing electron $P_{\epsilon l}(r)$ can be determined in various ways. The most basic way (which is the Hartree-Dirac-Slater method used by Verner et al. (1993)) of calculating $P_{\epsilon l}(r)$ is to treat the ionized electron as moving in the same effective central field both before and after ionization takes place. However, this treatment explicitly ignores the relaxation effect of the ionic core and correlation effects of the photoelectron and the ionic core electrons. It is inadequate to use this treatment for low energy (in the range from threshold to to about a few times of threshold) ionization and inner-shell ionizations where core relaxation and electron correlation effects are important. In our calculations, we include an essential part of many-electron correlation effect in a one-electron approximation by making a proper choice of the potential function for the outgoing photoelectron.

For outer shell ionization, we calculate $P_{\epsilon l'}(r)$ in the field of the next higher charge ion with the use of $P_{\epsilon l'}(r)$ in place of $P_{nl}(r)$ in the Hartree-Fock equation. For inner-shell ionization, part of the relaxation and correlation effects can be properly taken into account by using the HF potential of the outer shell electron in the initial bound state as the potential for the continuum orbitals. Figure 2 shows the 3s-subshell photoionization cross section of Ar I. Where circles represent the measurement of Marr et al. (1975); curve 1 is our calculational result with the HF potential for the outer shell electrons; curve 2 is our calculational result with the HF potential for the ionized subshell electrons; curve 3 is the

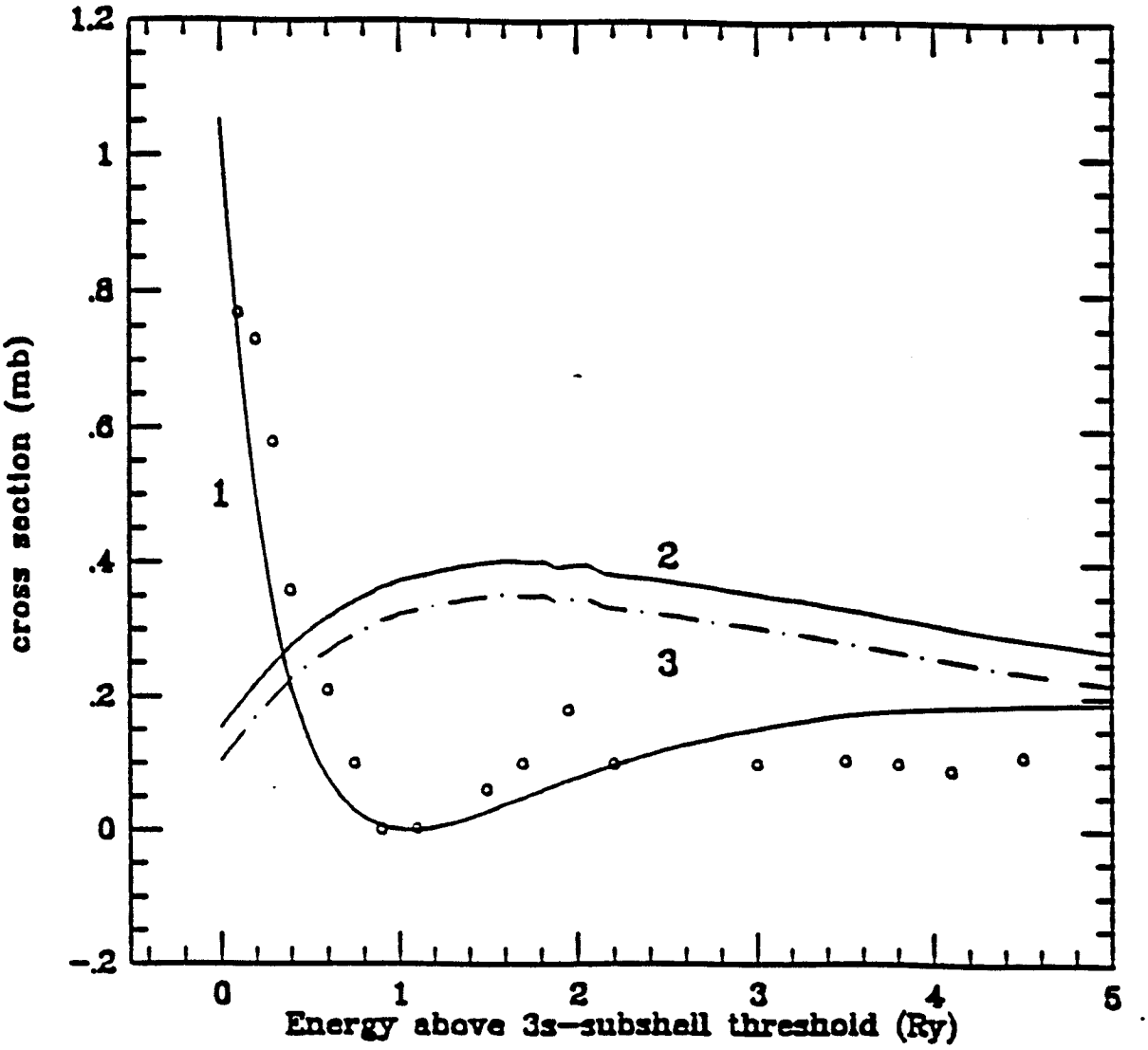

Figure 2. 3s-subshell photoionization cross section of ArI.
Circles: exparimental data of Marr et al.
Curve 1: data from this database.
Curve 2: result of HF calculation with complete relaxation approximation.
Curve 3: Cooper and Manson's HS calculation results.

HS result of Cooper and Manson (1969). The important feature here is the minimum in the cross section which is absent in curve 2 and 3. Curve 1 reproduces the experimental data well. This is a good example of correlation effect on photoionization cross sections. The good agreement of our calculation with the experimental data indicates that our treatment for continuum wavefunctions are adequate.

Comparisons of our calculated results with the smoothed Opacity Project calculations (Verner et al. 1996) and the recently published HDS photoionization cross section data calculated by Verner et al. (1993) are shown in Figure 3 to Figure 5. In Figure 3 we show the 2s and 2p cross sections for C I. In both our Hartree-Fock calculations and in the smoothed Opacity Project calculations, the shape and slope of the 2p-shell cross section is accurately predicted. The slope is shallow, so that there is no visible discontinuity at the 2s-shell threshold energy. The Hartree-Dirac-Slater calculations however, are less accurate near threshold, both in terms of the shape of the cross section and the normalization. Because of this inaccuracy, the HDS result shows a discontinuity at the 2s edge, which is not seen in the data. In Figure 4 we show that our HF calculation of the Si I cross section does a better job of reproducing the central energy of the resonance dip than does the HDS calculation. The same is true for the Ar I cross section shown in Figure 5, for which our HF calculation also reproduces the shape of the cross section just above the threshold energy quite well.

Generally speaking, the overall agreement of our Hartree-Fock calculations with the high-accuracy Opacity Project values is good. Our calculated cross sections in the regime near threshold of the outer shells may not be quite as accurate as those of Opacity Project calculations but our values far from threshold are better. The Opacity Project calculations are based on the higher level method such as the R-matrix method which are supposed to give more accurate low energy photoionization cross sections. In most cases, our results agree with the Opacity Project's results better than do the values calculated by Verner et al. (1993). The calculations of Verner et al. (1993) are based on the self-consistent Hartree-Dirac-Slater potential with the photoelectron wave functions determined under the frozen-core approximation. The frozen-core approximation completely omits the relaxation and correlation effects of core electrons which are supposed to be important to the cross sections near the ionization edges of each subshell. In our calculations, we include both the relaxation and correlation effects by properly choosing the potentials for outgoing photoelectrons. Therefore, our calculations are more accurate.

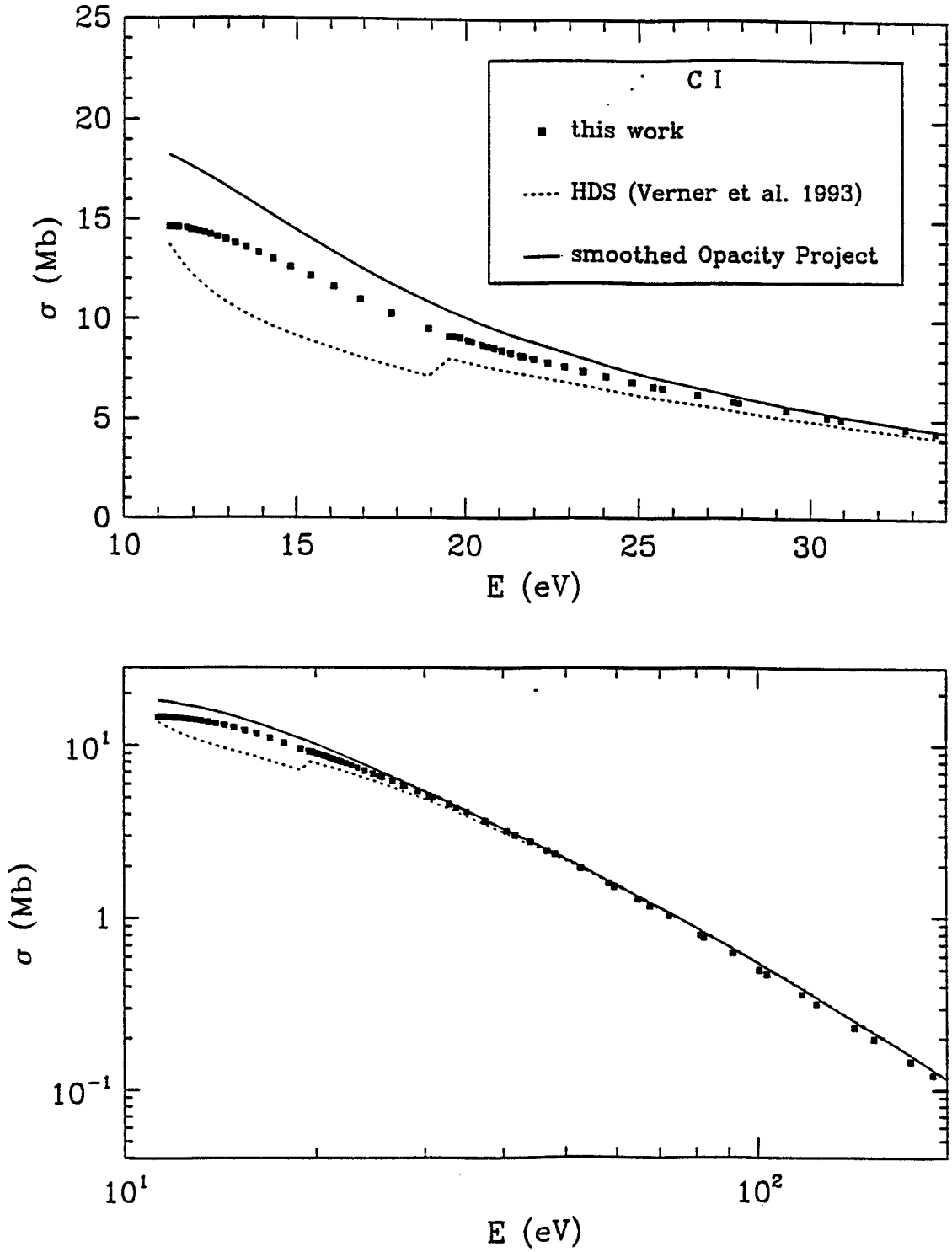

Figure 3. Total photoionization cross sections of CI.
Points: data from this database
Solid line: smoothed Opacity Project data
Dashed line: V&Y's calculations

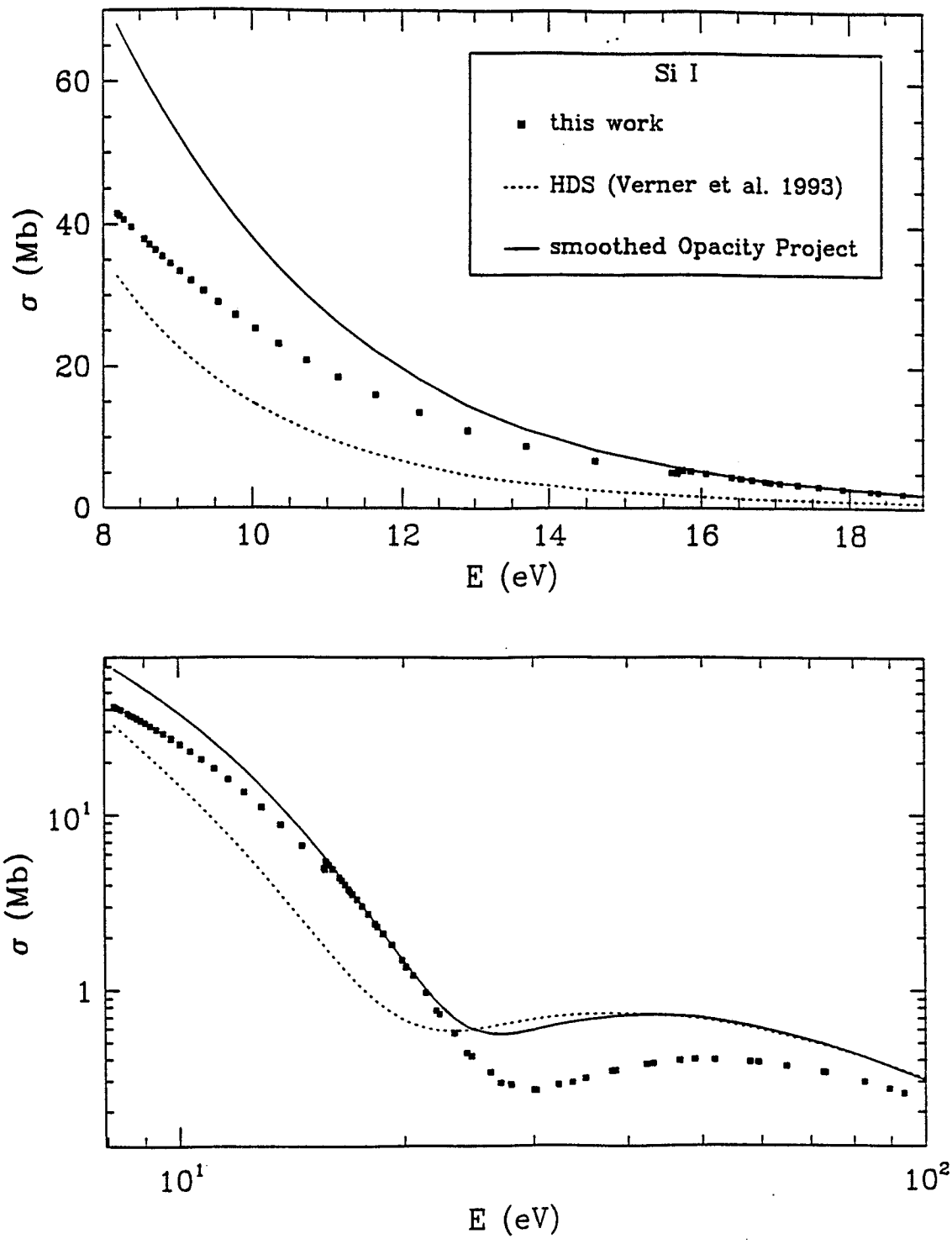

Figure 4. Total photoionization cross sections of SiI.
Points: data from this database
Solid line: smoothed Opacity Project data
Dashed line: V&Y's calculations

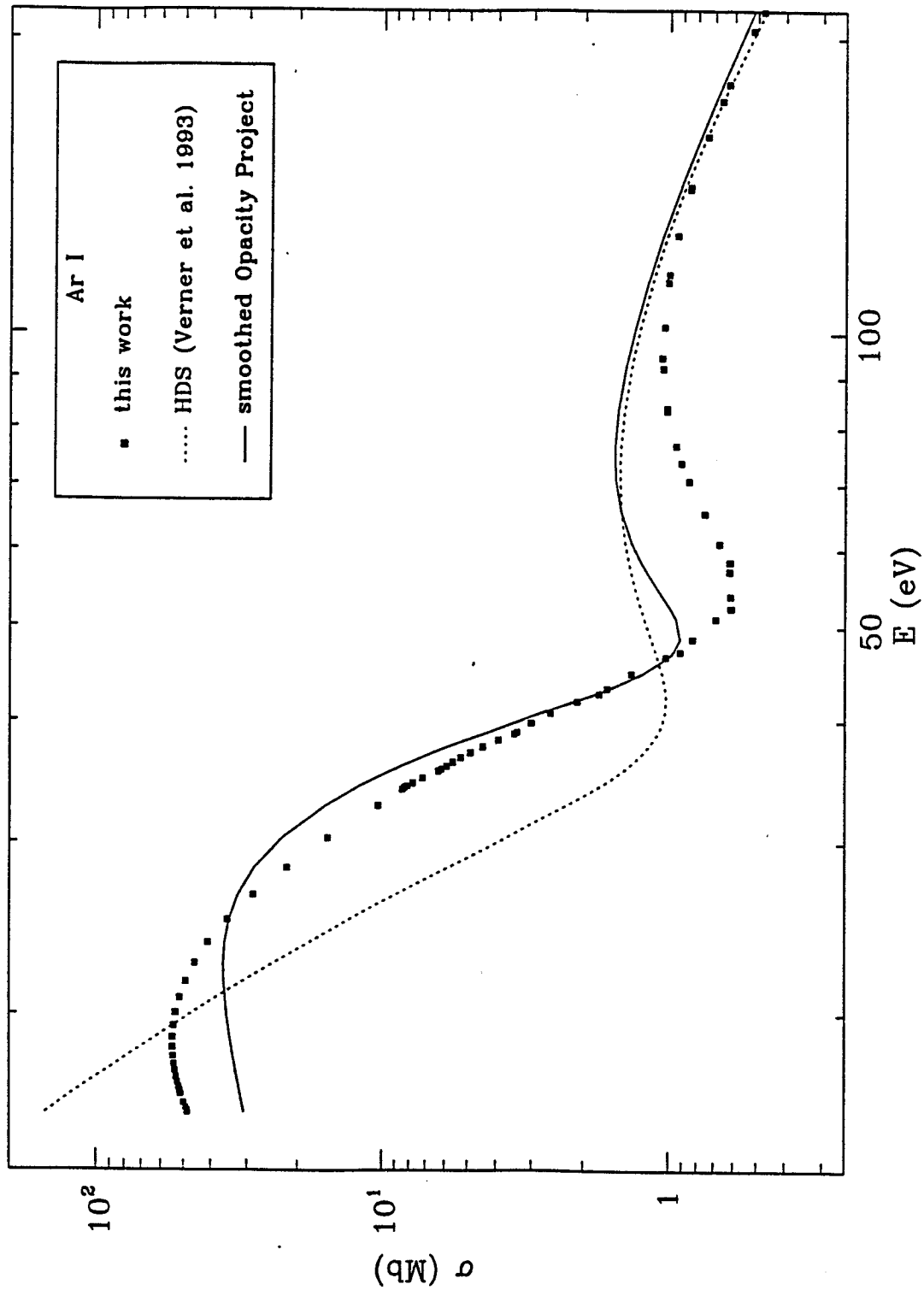

Figure 5. Total photoionization cross sections of ArI.
Points: data from this database
Solid line: smoothed Opacity Project data
Dashed line: V&Y's calculations

All the ionization thresholds in our database have been carefully evaluated. Experimental ionization potential data are used for the outer shell electrons. For inner shell electrons, the ionization thresholds are calculated with the used of multiconfiguration Hartree-Fock method under the complete relaxation approximation. We believe that the accuracy of all the ionization threshold values in our database is better than 1%.

In summary, the Hartree-Fock calculations of the photoionization cross sections we have performed provide a good match to the experimental data both near and far from the threshold energies of all subshells of ions ranging from neutrals up to highly ionized species. Our calculations also match the highly accurate near-threshold Opacity Project values quite well. And because our calculated cross sections are valid for all subshells and over a wide range of energies we avoid the problems of hybrid models (such as the HDS/Opacity Project compilation of Verner et al. 1996), in which the absolute values from the two methods will often disagree at the energy where the transition from one regime to the other occurs. The HF method is therefore more consistent in this intermediate energy range and also is more flexible when new cross sections (say for different ions) are required. Finally, given the difficulties and uncertainties in calculating photoionization cross sections, it is of benefit to the community to have a choice of methods and databases available.

(4) Data Fitting

In order to have a flexible, quick routine for returning the energy dependent cross sections for arbitrary combination of ions we need to fit continuous, analytic functions to the calculated cross sections tabulated at discrete energies. We explored various fitting functions including both purely empirical functions as well as functions based on the underlying physics. Ultimately, for conceptual reasons, we settled on the same function used by Verner and Yakovlev (1995) to fit their calculated cross sections. This five-parameter function is given by

$$\sigma_{nl}(E) = \sigma_0 F(y)\mathrm{Mb} \tag{3}$$

and

$$F(y) = [(y-1)^2 + y_w^2]^{-Q}(1 + (y/y_a)^{1/2})^{-P}, \tag{4}$$

where the dependent variable $y = E/E_0$, and E is the photon energy in eV, n is the principal quantum number, l is the subshell orbital quantum number ($s = 0$, $p = 1$, etc.), $Q = 5.5 + l - 0.5P$, and σ_0, E_0, y_w, y_a, and P are the five adjustable parameters. In general y_w, y_a, and P vary smoothly over atomic species for a given subshell, and the values of σ_0 and E_0 rescale the basic functional form of $F(y)$ for each species. In practice however, we find that for subshells of many species the fit is relatively insensitive to some combination

of the five fit parameters and we did not make an effort to use values of the parameters that allowed for a smooth variation with species. Rather we chose values that maximized the goodness of fit.

The advantage of this fitting function over, say, high order polynomials which actually gave slightly better statistical fits, is that each of the five parameters of the functions described by the above equations has a physical meaning. Many cross sections have resonant dips above the threshold energy. The location of such resonances are given by the E_0 parameter and their widths are given by y_w. At very high energies the non-relativistic asymptote, $\sigma_{nl}(E) \propto E^{-3.5-l}$ is reproduced, and at intermediate energies $F(y) \propto y^{-Q}$. The boundary between these two regimes is dictated by the value of y_a. Note that for partial cross sections with no resonant dips E_0 will be less than the threshold energy.

Using this fitting function we were able to achieve generally good fits to our calculated cross sections from threshold up to, in most cases, 50 keV. We fit the calculations using Levenberg-Markwardt minimization of the χ^2 statistic, assuming uniform errors. For each fit we calculated the root mean square deviation and the maximum deviation. In general the rms deviations were a few percent or less and the maximum deviation was rarely more than 10 percent. For outer shells of some high-Z neutrals the fits were several times worse, although the maximum deviations never exceeded 25 percent. The quality of these functional fits is not as good as that reported by Verner and Yakovlev (1995), perhaps due to our non-relativistic treatment. However the errors in the fitting functions are small compared to disagreement between calculated (and often between experimental) values in the literature, and are unimportant for current astrophysical applications.

(5) Applications

Our fitted energy-dependent cross sections will be useful to many astrophysicists, engineers, and physicists for observational, experimental, and theoretical work. Cross sections of individual subshells or ions will be used by experimentalists comparing laboratory derived values to theory, and by other researchers studying specific ions. As in any complex field it is very useful to have data and calculations from multiple sources using different methods to evaluate the importance of different effects and to estimate the uncertainties of the calculated values (see section 3).

In astrophysics, cross sections of individual ions are needed *e.g.* to make nebular models, to assess the optical depth of interstellar and intergalactic gas, to model stellar atmospheres, and AGN broad-line regions, and to properly analyze observations of these objects. For analyzing the current generation of low and moderate resolution high-

energy astrophysical data *global* models of the photoionization cross sections of cosmically abundant plasmas with a mixture of ionization stages are needed. Our cross section tabulation, in conjunction with the tabulation of ionization balance models for a wide range of physical conditions, can be used in standard X-ray data analysis packaged like XSPEC or PROS (or even off-line) to analyze data from a wide variety of astrophysical objects much more accurately than is commonly done now.

Most of the testing we have performed thus far involves hot star winds. We have used the photoionization cross sections computed for this project to fit the combined *EUVE* and *ROSAT* data sets of ϵ CMa (Cohen et al. 1996) and also to fit the *ROSAT* spectra of a large number of B stars (Cohen, Cassinelli, & MacFarlane 1997). In both of these studies we found that the derived X-ray and EUV properties of the stars in question differed markedly when we used photoionization cross sections which were based on a realistic ionization structure in the wind material overlying the sites of X-ray emission. In several cases we were even able to use the X-ray data to distinguish among different ionization, and hence attenuation models. The quality of the *ROSAT* and *EUVE* data was not good enough to put constraints on the abundances of specific ions, but it was sufficient to constrain the overall ionization levels.

(6) Conclusions

We have successfully established an X-ray analysis database of photoionization cross sections including variable ionization. This database provides to the high-energy astrophysics community a tabulation of energy-dependent photoionization cross sections for all ionization stages of 17 common elements. This includes hundreds of ionization stages from neutrals to hydrogen-like heavy elements. We also provide tabulation of ionization distributions based both on coronal ionization equilibrium and selected photoionization conditions to enable users to parameterize the degree of ionization in the absorbing medium in a simple manner. The database is available to all the scientists in the community. Interest users can directly contact us through email: wang@atom.neep.wisc.edu. We will provide all the technical details which include (1) a users' guide, (2) reference manual, (3) installation procedures, (4) Makefiles, and (5) test data and procedures. These products will be available to the community via our www site sometime during summer 1997, and our fitting package will be included in the next release of XSPEC.

References

Cohen, D. H., Cohen, R. G., MacFarlane, J. J., Owocki, S. P., Cassinelli, J. P., & Wang, P. 1996, ApJ, 460, 506.

Cohen, D. H., Cassinelli, J. P., & MacFarlane 1997, ApJ, in press.

Cooper, J. W., & Manson, S. T., 1969, Phys. Rev, 177, 157.

Corcoran, M. F., Swank, J. H., Serlemitsos, P. J., et al. 1993, ApJ, 412, 792.

Cowan, R. D. 1981, *The Theory of Atomic Structure and Spectra*, University of California Press, Berkeley, 1981.

Daltabuit, E., & Cox, D. 1972, ApJ, 177, 855.

Ferland, G. J., University of Kentucky, Department of Physics and Astronomy, Internal Report.

Henke, B. L., Lee P., Tanaka, T. J., Shimabukuro, R. L., & Fujikawa, B.K 1982, Atomic Data Nucl. Data Tables, 27, 1.

Krolik, J. H., & Kallman, T. R. 1984, ApJ, 286, 366.

Lloyd, H. M., O'Brien, T. J., Bode, M. F., Predahl, P., Schmitt, J. H. M. M., Trumper, J., Watson, M. G., & Pounds, K. A. 1992, Letters to Nature, 356, 222.

Marr, G. V., et al. 1975, J. Phys. B8, 2638.

Petre, R., Mushotzsky, R. F., Krolik, J. H.,& Holt, S. S. 1984, ApJ, 280, 499.

Seaton, M. J. 1987, J. Phys. B20, 6363 (Opacity Project; OP).

Verner, D. A., Ferland, G. J., Koritsa, K. T., & Yakovlev, D. G. 1996, ApJ, 465, 487.

Verner, D. A., & Yakovlev, D. G. 1995, A&A Supp. Series, 109, 125.

Verner, D. A., Yakovlev, D. G., Band, I. M., & Trzhaskovskaya, M. B. 1993, Atomic Data Nucl. Data Tables, 55, 233.

Williams, R. E. 1989, in *Physics of Classical Novae*, IAU coll 122, eds. A. Cassatella, R. Viotti, 215.